Nanoelectromechanical systems based on multi-walled nanotubes: nanothermometer, nanorelay and nanoactuator

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Abstract

We report on three new types of nanoelectromechanical systems based on carbon nanotubes: an electromechanical nanothermometer, a nanorelay and a nanomotor. The nanothermometer can be used for accurate temperature measurements in spatially localized regions with dimensions of several hundred nanometers. The nanorelay is a prototype of a memory cell, and the nanoactuator can be used for transformation of the forward force into the relative rotation of the walls. Relative motion of the walls in these nanosystems is defined by the shape of the interwall interaction energy surface. *Ab initio* and semi-empirical calculations have been used to estimate the operational characteristics and dimensions of these nanosystems.

1 Introduction

Unique properties of carbon nanotubes, such as free sliding and rotation of the walls and metallic conductivity, allow using the walls of nanotubes as movable elements and elements of electric circuit in nanoelectromechanical systems (NEMS). An example of such applications is a nanotube-based nanomotor which has been produced recently [1, 2]. A set of NEMS based on relative motion of the walls of nanotubes, such as a nanospring [3], a nanoswitch [4] and a gigahertz oscillator [5] have been suggested in the literature. A number of nanorelays with one electrode made of a carbon nanotube have also been considered [6, 7, 8]. A new type of NEMS in which the relative motion of the walls is controlled by the shape of the interwall interaction energy surface has been proposed in [9, 10] as a nanodrill, in [11] as a tension nanosensor and in [12, 13] as rotational nanobearings with fixed position along the axis. In this paper, we propose three new NEMS of this type: an electromechanical nanothermometer, a nanorelay with all electrodes made of nanotubes, which can also be used as a memory cell, and a nanoactuator for transformation of forward force into relative rotation of the walls.

2 Methods of calculations

The density functional theory supercell code within the local density approximation (AIMPRO [14]) has been used to calculate the interwall interaction energy and the barriers to the relative sliding of the walls for

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the (5,5)@(10,10) and (6,6)@(11,11) double-walled carbon nanotubes (DWNTs). The details of the method can be found in [13, 15]. Within AIMPRO, the pseudowave functions are described by 4 atom-centered Gaussian functions per atom expanded in spherical harmonics up to l=1, with the second smallest exponent expanded to l=2. The supercell consists of 60 and 68 carbon atoms for the (5,5)@(10,10) and (6,6)@(11,11) DWNTs, respectively. The Brillouin Zone sampling has been performed using 18 special k-points in the direction of the nanotube axis. Non-local, norm-conserving pseudopotential and the standard Perdew-Wang exchange-correlation functional [16] have been used. Minima in the total energy are found using a conjugate gradient scheme to an accuracy of 1 μeV/atom. Positions of all atoms in the isolated (5,5), (6,6), (10,10) and (11,11) walls have been optimized.

Structures of the caps of the nanotubes used as the electrodes of a nanorelay have been calculated using the Q-Chem 2.1 quantum chemistry package [17]. The 6-12 Lennard-Jones potential U=$4\epsilon((\sigma/r)^{12}-(\sigma/r)^{6})$ has been used for calculation of the interaction between the electrodes of a nanorelay. Parameters σ=3.44 Åand ϵ=$2.62\cdot10^{-3}$ eV [18]) have been used for the interaction between carbon atoms, and σ=2.039 Å, ϵ=0.14438 eV [19] for the interaction between carbon and copper atoms.

3 Nanoelectromechanical systems

3.1 Electromechanical nanothermometer

A new concept of an electromechanical nanothermometer is based on the interaction and relative motion of the walls of carbon nanotubes. Temperature measurements are carried out through the measurements of the electrical conductance of the walls as a function of their relative displacement. Relative position of the walls of a nanotube depends on and changes with the temperature due to the thermal vibrations of the walls. The probability of the relative displacement of the walls, $p(q)$, is defined by the energy of their interaction, $U(q)$, as $p(q) \sim exp(-U(q)/kT)$. For a given temperature, the total conductance, $G_{tot}(T)$, can, therefore, be found as the expectation value of the conductance at a fixed position of the walls, $G(q,T)$ [20]

$$G_{tot}(T) = \frac{\int\limits_{-\infty}^{\infty} G(q,T)\exp(-U(q)/kT)dq}{\int\limits_{-\infty}^{\infty} \exp(-U(q)/kT)dq}. \quad (1)$$

Equation 1 takes into account contributions from the thermal vibrations of the walls.

The working conditions for the electromechanical nanothermometer are the following: $G(q,T)$ depends significantly on the coordinates q (condition A); $G(q,T)$ depends weakly on the temperature T (condition B) (contributions from phenomena other than the thermal vibrations of the walls are insignificant); amplitude of the thermal vibrations is large enough to provide the main contribution to the temperature dependence of the total conductivity $G_{tot}(T)$ (condition C); amplitude of the thermal vibrations is still small for the relative displacements of the walls to upset the normal operation of the system (condition D).

A model implementation of the nanothermometer is based on the (6,6)@(11,11) DWNT (Figure 1). The conductance of the (6,6)@(11,11) DWNT depends significantly on the relative position of the walls in both telescopic and shuttle systems [21] and changes due to the thermal vibrations of the walls. Therefore, the condition A is fulfilled. Experimental studies of [22] show that the conductance of single-walled carbon nanotubes depends weakly on the temperature in the region of T >50 K. Theoretical studies of [23] conclude that for DWNTs with fixed walls it depends weakly on the temperature for T >100 K. Thus, the condition B is also satisfied in these temperature regions.

The dependence of both the interaction energy of the walls of a nanotube and the conductance on the displacement of the walls is uniquely determined by the symmetry of the (6,6)@(11,11) DWNT. $U(q)$ and $G(q)$ show some common features, for example, they have the same period of oscillation and the extrema in both functions coincide. Moreover, the dependence of the interwall interaction energy and the conductance

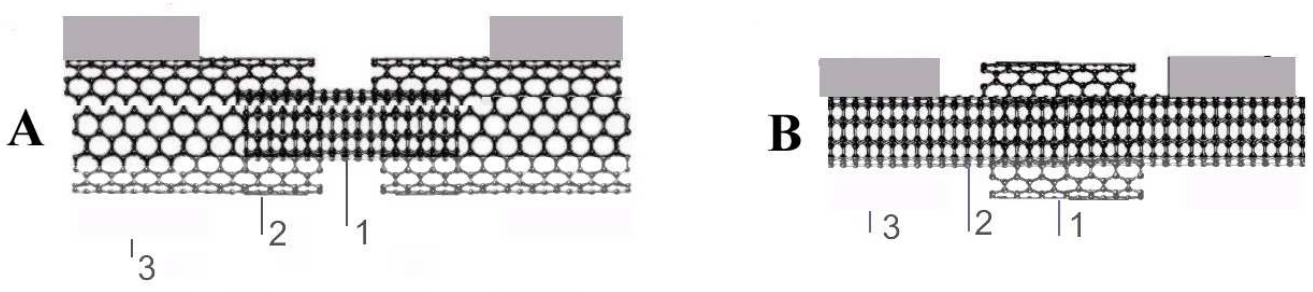

Figure 1: Schematic of an electromechanical nanothermometer based on DWNT. A: a shuttle nanothermometer with the movable inner wall, B: a telescopic nanothermometer with the movable outer wall. 1 is the movable wall, 2 is the fixed wall with the attached electrodes 3.

on the angle of relative rotation of the walls is negligible due to incompatibility of the rotational symmetries of the (6,6) and (11,11) walls.

In the absence of diffusion of the short wall, integration in equation (1) can be performed near the bottom of the potential well of the interwall interaction energy $U(q)$. This region can be interpolated as [24]

$$U(q') = U_1 + \frac{\pi \Delta U_q}{\delta_q^2} q'^2, \tag{2}$$

where U_1 is the interwall interaction energy of the ground state, ΔU_q is the energy barrier between the minima of $U(q)$, δ_q is the period of displacement of the walls between the minima, and q' is a displacement of the movable wall from the position which defines the ground state. For small values of q', $G(q', T)$ can be interpolated as [24]

$$G(q') = G_1(T)(1 + \gamma q'^2), \tag{3}$$

where G_1 is the conductivity of DWNT in the ground state. The value of γ for the overlap of the walls of 2.45 nm can be extracted from the Figure 3 of [21] as $\gamma \sim$850 Å^{-2}.

Substitution of (2) and (3) into (1) leads to the following expression for the dependence of the conductance of the nanothermometer on the temperature

$$G(T) = G_1(T)(1 + \frac{\gamma \delta_q^2 kT}{\pi \Delta U_q}) = G_1(T)(1 + HT). \tag{4}$$

Here the energy barrier ΔU_q for the (6,6)@(11,11) DWNT has been calculated *ab initio* and for the overlap of the walls of 2.45 nm it has the value of 1.96 eV. Therefore, for T=300 K, the value of HT in (1) is about 45 and this ensures the fulfillment of the condition C. For the condition D to be satisfied, the displacement of the shuttle as a result of diffusion has to be less than the distance between the electrode and the shuttle. The minimum length between the electrodes of the shuttle nanothermometer which operates during 100 years without a failure is estimated as 38 nm using the *ab initio* results [25] for the diffusion coefficient of the walls of (6,6)@(11,11)DWNT. The nanothermometer can be calibrated with the use of a thermocouple, and since the temperature measurement is based on conductance measurement, the same order of accuracy as in the case of thermocouple using can be achieved (for example, the accuracy of measurements at room temperature is about 0.1 K for copper-constantan and chromel-alumel thermocouples).

3.2 Nanorelay

The essential working condition for a nanosystem to operate as a relay is the presence of two minima in the interaction energy of its components (positions 'on' and 'off'), or so called bi-stability. The new type of nanotube-based nanorelay has been proposed recently (Figure 2A). Here we proposed new schemes of

nanorelays of this type (Figures 2B and 2C). Their operation is fully determined by the the forces applied to the movable inner wall 1. These forces are the attraction force, F_a, of the Van der Waals interaction between the electrodes; the electrostatic force, F_e, between the electrodes 3 and 4 (Figures 2A and 2B) or between the electrode 3 and the control electrode 5 (Figure 2C); and the forces of the interwall interaction, such as the capillary force F_c, which retracts the inner wall, and the static friction force F_f.

For the (5,5)@(10,10) DWNT, the capillary force F_c is estimated in [13] as 0.625 nN. The results for calculations of the interaction between the electrodes are presented in Table 1. According to the *ab initio* [15] and semiempirical [12] calculations, the friction force F_f is approximately zero for DWNTs with incommensurate or/and chiral walls. If the condition for bi-stability, $F_a > F_c$, is satisfied then the nanorelay can be used as a memory cell of the external storage. If one of the electrodes of the nanorelay is made of a DWNT with incommensurate or chiral walls, the condition for bi-stability can only be achieved if the second electrode is flat (see Figure 2A). An 'all-carbon' nanorelay with both electrodes made of carbon nanotubes is shown in Figure 2B. In the case of small friction force F_f, this nanorelay is stable in position 'on' only if the voltage is applied. Therefore, it can be used as an easy-to-operate memory cell of the on-line storage (see Figure 2D).

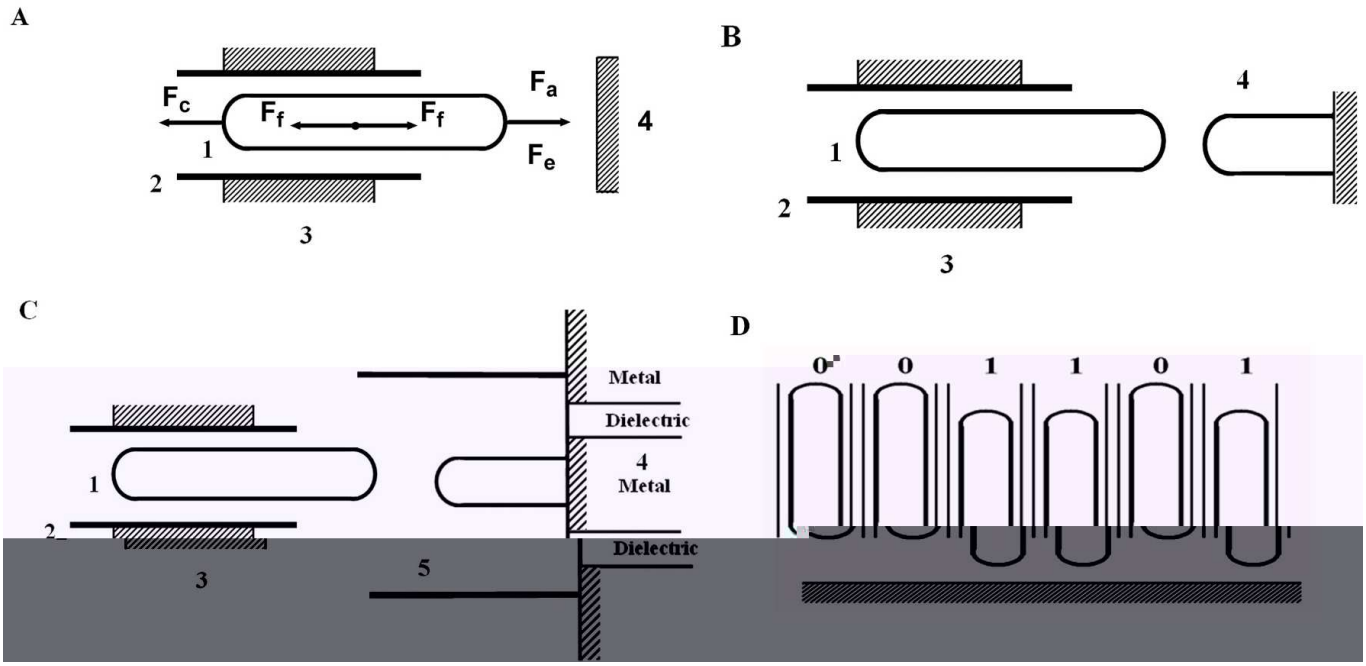

Figure 2: Schematics of memory cells based on DWNTs (in position 'on'). A: a memory cell with a flat second electrode; B: an 'all-carbon' memory cell with a carbon nanotube attached to the second electrode; C: an 'all-carbon' memory cell with a control electrode made of a nanotube. 1 is the movable inner wall; 2 is the fixed outer wall; 3, 4 and 5 are the first, second and the control electrodes. Figure D shows an example of the storage produced from memory cells.

In the case of DWNTs with nonchiral commensurate walls, the friction force F_f is significant [12, 15]. For the (5,5)@(10,10) DWNT, the dependence of the force F_f on the overlap of the walls, l_{ov}, can be described as $F_f = Al_{ov}\cos(2\pi l_{ov}/\delta_q)$, where $A = 0.01$ N/m [13]. The analysis of the balance of forces in 'all-carbon' nanorelay shows that for the critical overlap $l_c = 4$ nm, the sum of the interwall static friction force and the attraction force of the Van der Waals interaction between the electrodes, $F_f + F_a$, has to be greater than the capillary force F_c. If the overlap of the walls is greater than the critical value, $l_{ov} > l_c$, the nanorelay can be bi-stable.

The condition $l_{ov} > l_c$ is not sufficient for the successful operation of the 'all-carbon' nanorelay as a

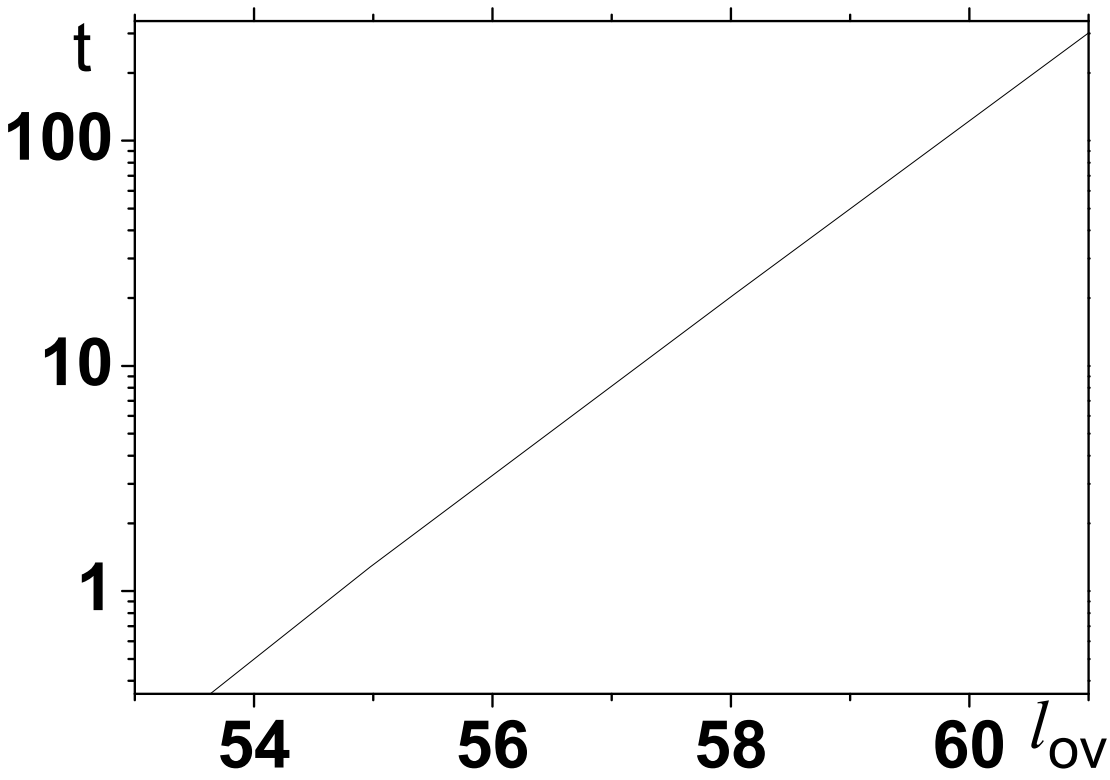

Figure 3: The dependence of the lifetime of the 'all-carbon' nanorelay in position 'on' on the overlap of the walls. The nanorelay contains the (5,5)@(10,10) DWNT as the first electrode and the (5,5) nanotube as the second electrode.

memory cell of the external storage. The energy barrier between positions 'on' and 'off' can be, in principle, overcome as the result of the thermal diffusion of the inner wall 1. The probability of this to happen is determined by the Arrhenius formula $p = \Omega \exp(-\Delta U/kT)$, where Ω is the frequency multiplier. According to the molecular dynamics simulation of the reorientation of shells of the $C_{60}@C_{240}$ nanoparticle [26], the frequency multiplier is about an order of magnitude greater than the frequency of small oscillations near the minimum of the intershell interaction energy. The dependence of the lifetime, $t = p^{-1}$, of the 'all-carbon' nanorelay in position 'on' on the overlap of the walls is shown on in Figure 3.

For the case of a nanorelay with the control electrode made of a carbon nanotube (Figure 2C), the electrostatic force F_e acting on the (5,5) movable wall has been calculated. The diameter of the movable wall, as well as the control electrode, is taken to be 3 nm as the armatures of cylindrical capacitor. Assuming the friction force F_f is negligible, the voltage of the switching between positions 'off' and 'on' can be determined by the condition $F_e > F_c$ and estimated to be about 6 V. In this case, the voltage needed to hold the nanorelay in position 'on' is about 4.8 V.

Table 1: Characteristics of the interaction between the electrodes of the nanorelay: U_{min} (in eV) is the minimum value of the interaction energy between the electrodes, R_{min} (in Å) is the distance between the electrodes which corresponds to the minimum of the interaction energy; F_a^{max} (in nN) is the maximum attraction force between the electrodes.

second electrode	U_{min}	R_{min}	F_a^{max}
graphite	-0.914	3.153	0.683
copper	-35.69	1.879	42.32
(5,5) nanotube	-0.259	3.345	0.233

3.3 Nanoactuator

A nanoactuator has been designed for transformation of the forward force into the relative rotation of the walls. Schematic of the nanoactuator is shown in Figure 4. The wall 1 of the nanotube is fixed making a stator. Position of a rotor (the walls 2 and 3) is also fixed. The walls 3 and 4 make up a bolt-nut pair which converts the motion driven by an axially directed force applied to the wall 4 into the rotation of the rotor. It has been shown in [27, 28] that the bolt-nut pair can be a DWNT with periodically positioned defects.

The first of the essential working conditions for the nanoactuator is defined by the motion of the walls 1 and 2, which constitute a rotational nanobearing. This condition states that the barrier to the rotation of the walls 1 and 2 has to be low and the barrier to the sliding axial motion of these walls has to be high. This condition is satisfied if both 1 and 2 are commensurate achiral walls with incompatible rotational symmetry [12, 13].

The second of the essential working conditions for the nanoactuator is defined by the motion of the walls 3 and 4, which constitute a bolt-nut pair. If a short impulse of the force directed along the axis is applied to the wall 4, this wall acquires the kinetic energy sufficient to overcome the barrier E_1 to the motion of the walls 3 and 4 along the line of the thread. However, the energy will not be large enough to overcome the barrier E_2 to the motion of the walls 3 and 4 across the line of the thread, i.e.

$$\frac{M\mathbf{V}^2\sin^2\chi}{2} > E_1, \qquad \frac{M\mathbf{V}^2\cos^2\chi}{2} < E_2, \tag{5}$$

where M and $\mathbf{V}$ are the mass and velocity of the wall 4, and χ is the angle of the thread. The inequalities (5) are fulfilled if $\cot^2\chi < E_2/E_1 = \beta$ where β is the depth of the thread as given in [9, 10]. Evidently, if the angle χ of the thread is greater than 45 degrees than the nanoactuator can operate with any depth of the thread. The charges on the edges of the wall 4 can be produced by chemical adsorption.

The conservation of the angular momentum of the nanoactuator gives the minimum length L_3^{min} of the wall 3 for which the rotation at an angle ξ becomes possible

$$L_3^{min} = \frac{L_4^2R_4^2}{L_4R_4^2 + \xi(R_2^3 + R_3^3)\sin\chi}, \tag{6}$$

where L_4 is the length of the wall 4; R_2, R_3 and R_4 are the radii of the walls 2, 3 and 4, respectively. The operation time of the proposed nanorelay and nanoactuator can be the same order of magnitude as oscillation period $10 - 100$ ps of nanotube-based gigaherts oscillator [5].

4 Conclusive remarks

We proposed three new nanotube-based NEMS: a nanothermometer, a nanorelay with 'all-carbon' electrodes and a nanoactuator. A considerable progress has been recently achieved in the nanotechnology techniques in the field of production of NEMS. A nanomanipulator can be now attached to MWNT in order to move

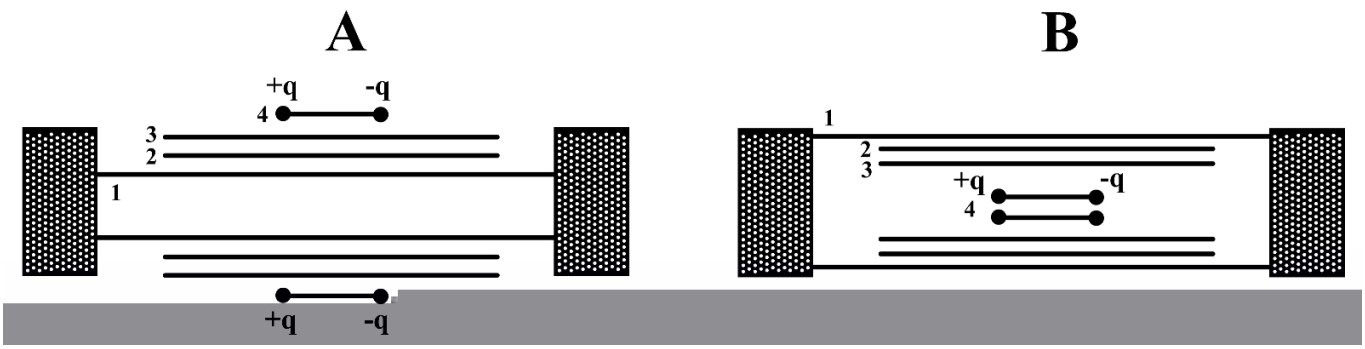

Figure 4: Schematic of a nanoactuator. A: a nanoactuator with the inner wall 1 as a stator, B: a nanoactuator with the outer wall 1 as a stator. The walls 1 and 2 comprise the rotational nanobearing, the walls 3 and 4 are the bolt-nut pair with the thread-like shape of the interwall interaction energy.

individual walls [3], manipulation with nanotubes is routinely possible [29], the caps of the walls can be removed [30], nanotubes can be cut into pieces of desirable length [31], the techniques for unambiguous determination of chirality of the walls have been successfully demonstrated [32]. All these gives us a cause for the optimism that the proposed NEMS will be produced in the near future.

5 acknowledgement

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